Gallium Nitride Crystal Growth Kinetics from Selective-Area Growth Experiments and 3-D Morphology Evolution Model

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Motivation—Crystals that grow in nature usually have convex features that form as the crystal grows outward. The fastest growing faces grow to extinction, and the crystal is then bounded by the slowest growing faces. The Wulff construction is a polar plot of the facet-orientation-dependent growth rate. At long time the shape of a grown crystal will match the Wulff shape. For growth of *concave* features, the rules change. The fastest growing faces actually grow to dominance, rather than disappear. We have developed a new approach to measure the intrinsic growth rates of the fast-growing crystal faces in GaN using special patterning in an Epitaxial Lateral Overgrowth (ELO) mask. Concave growth templates are created lithographically to force the "inward" growth geometry The Princeton group (Du and Srolovitz) are developing a 3-D crystal facet evolution model to extract the intrinsic GaN crystal growth kinetics of orientations "missing" from the Wulff shape.

Accomplishment—A representative plan-view scanning electron micrograph (SEM) image is shown in Fig. 1(a). The shape of the original exposed growth zone is shown as the blue hexagonal feature in Fig. 1(b), and as the yellow outline in the each of the images. The unexposed interior and outer regions are covered with a dielectric mask. GaN ELO occurs selectively only on the exposed feature, growing both laterally over the mask and vertically. Shown in Figs. 1(c)-(f) are model simulations of the growth as time proceeds. The and equivalent facets, red faces in the figure, are $(11\bar{2}2)$ aligned parallel to the edges of the hexagonal pattern, and are the fastest growing of the three major faces illustrated. As the ELO feature grows outward from the pattern, the faces grow to extinction. The slowest growing faces, $(11\bar{2}2)$ colored brown in the figure and $(1\bar{1}01)$ aligned 30° from the faces, become larger and bound $(11\bar{2}2)$ the *outside* perimeter at long time. This illustrates the expected behavior for growth of convex features, as seen in the SEM image and calculation, Figs. 1(a) and 1(f). The feature also grows rapidly in the vertical direction, causing the exposed basal plane (0001) to shrink with time. Figure 1(a) shows that inside the feature, i.e., for concave growth, the fast-growing faces are dominant, exactly $(11\bar{2}2)$ opposite of the situation outside the feature. It is evident that the model captures the qualitative aspects of the crystal evolution at the convex and concave corners. However, the center portion of the structure has filled before the outside portion has grown to a hexagon, indicating that the facet rate constants in the simulation are not in the correct ratio.

Significance—Sandia has developed a related GaN defect-reduction technique called Cantilever Epitaxy (CE). We have shown that vertical threading dislocations can be reduced by proscribed variation of the crystal facet morphology during growth. A fundamental understanding of GaN crystal growth kinetics, and especially how it varies with temperature, provides quantitative guidance to control and manipulate the crystal morphology during CE growth and coalescence. Understanding the crystal coalescence in the interior of such features will also give us insight into the coalescence of polycrystalline GaN during the growth and ripening of the initial nucleation layer during heteroepitaxy.

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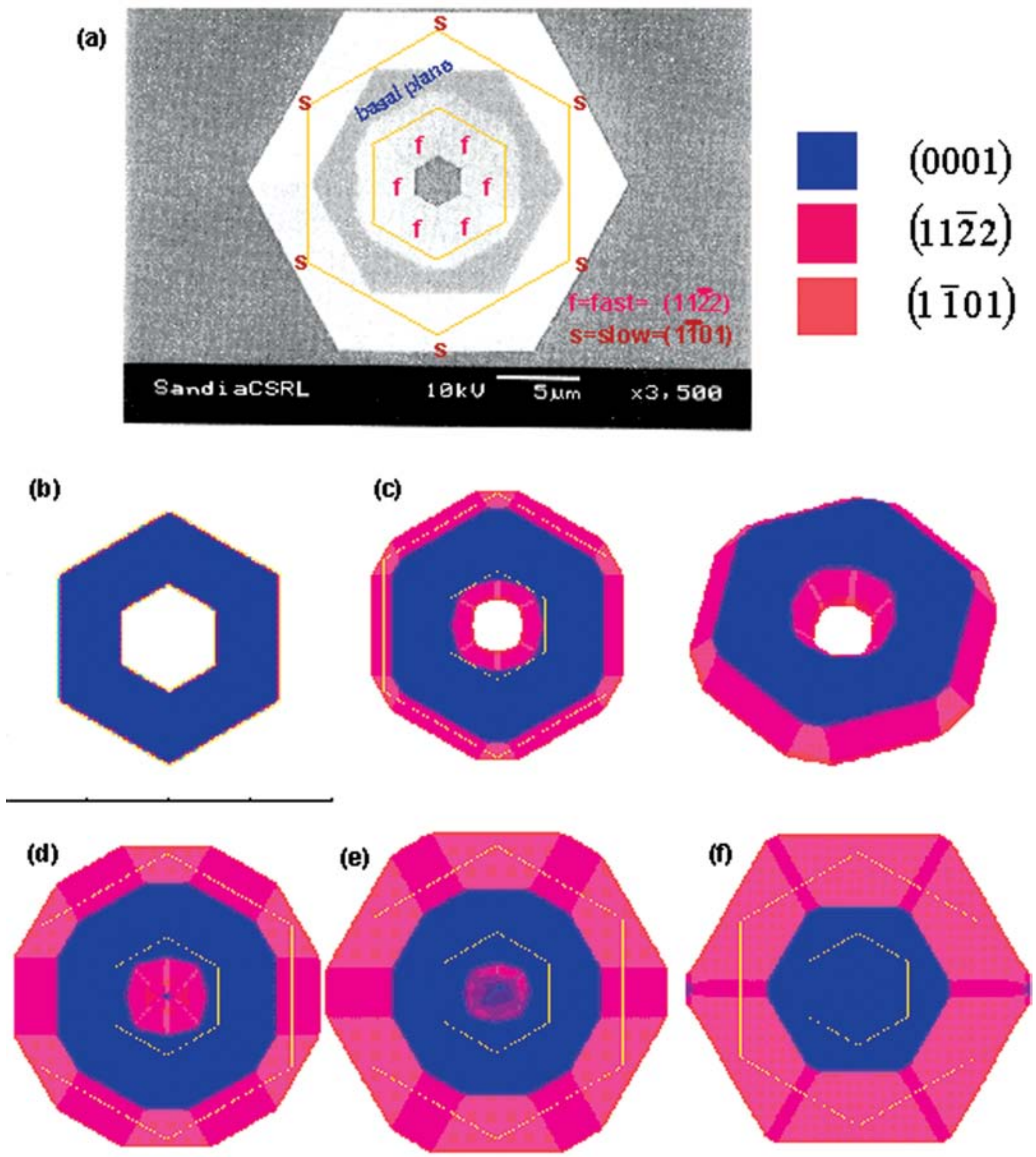

Figure 1. (a) Scanning electron micrograph (SEM) image of a GaN ELO feature grown from a hexagonal annular pattern. Fast-growing (11$\bar{2}$2) facets are labeled with "f," slower-growing (1$\bar{1}$01) faces are labeled with "s," and the (0001) basal plane appears as grey, in the plane of the image. The original exposed pattern is shown in blue in part (b). The calculated feature shape at early time is shown in plan view and perspective in part (c). Identification of the crystal facets by color is given at the top right portion of the page. Parts (d) through (f) show how the ELO feature shape evolves as growth proceeds. The simulation clearly shows the fast-growing (11$\bar{2}$2) faces growing to extinction at the convex corners, i.e., the outer boundaries of the crystal.